

Chemical Safety Data Sheet MSDS / SDS

1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile SDS

Revision Date:2024-04-25 Revision Number:1

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name: 1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile

CAS: 7027-11-4

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 4, Oral

Skin sensitization, Category 1

Specific target organ toxicity - repeated exposure, Category 2
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H302 Harmful if swallowed
H317 May cause an allergic skin reaction
H373 May cause damage to organs through prolonged or repeated exposure
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P273 Avoid release to the environment.

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P317 If skin irritation or rash occurs: Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P319 Get medical help if you feel unwell.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile
Common names and synonyms:	1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile
CAS number:	7027-11-4
EC number:	-
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison

Control Center immediately.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

Specific hazards arising from the chemical

no data available

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Melt.
Colour:	no data available
Odour:	no data available
Melting point/freezing point:	62 °C.
Boiling point or initial boiling point and boiling range:	279.88 °C. Atm. press.:1 013.25 hPa. Remarks:Boiling temperature extrapolated.;Ca. 145 - 150 °C. Atm. press.:16 hPa. Remarks:Value reasonably corresponds with Beilstein.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	157 °C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature:	465 °C. Atm. press.:1 013.25 hPa.
Decomposition temperature:	no data available
pH:	no data available

Kinematic viscosity:	no data available
Solubility:	In water: 4.91 g/L. Temperature:20 °C. pH:8 - 8.1.
Partition coefficient n-octanol/water:	log Pow = 1.6. Temperature:23 °C. Remarks:Main component.;log Pow = 1.8. Temperature:23 °C. Remarks:Isophorone.
Vapour pressure:	0.001 hPa. Temperature:20 °C.;0.038 hPa. Temperature:50 °C.
Density and/or relative density:	943.1 g/L. Temperature:80 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 365 mg/kg bw.

Inhalation: no data available

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - > 10 - 22 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - > 100 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 350 mg/L - 72 h.

Toxicity to microorganisms: TT = toxic threshold concentration - Pseudomonas putida - 1 380 mg/L - 17 h.

Persistence and degradability

no data available

Bioaccumulative potential

no data available

Mobility in soil

no data available

Other adverse effects

no data available

SECTION 13: Disposal considerations**Disposal methods**

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: No
IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Not Listed.

EC Inventory

Not Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any